

PATENT COOPERATION TREATY

PCT

INTERNATIONAL PRELIMINARY REPORT ON PATENTABILITY

(Chapter II of the Patent Cooperation Treaty)

(PCT Article 36 and Rule 70)


REC'D 07 DEC 2005

Applicant's or agent's file reference 9013.009-304	FOR FURTHER ACTION		See ANNEX PCT/PEA/416	PCT
International application No. PCT/US2004/035444	International filing date (day/month/year) 27.10.2004	Priority date (day/month/year) 27.10.2003		
International Patent Classification (IPC) or national classification and IPC G01N23/207				
Applicant SSCI, INC. et al.				

- This report is the international preliminary examination report, established by this International Preliminary Examining Authority under Article 35 and transmitted to the applicant according to Article 36.
- This REPORT consists of a total of 7 sheets, including this cover sheet.
- This report is also accompanied by ANNEXES, comprising:
 - ☐ sent to the applicant and to the International Bureau) a total of sheets, as follows:
 - ☐ sheets of the description, claims and/or drawings which have been amended and are the basis of this report and/or sheets containing rectifications authorized by this Authority (see Rule 70.16 and Section 607 of the Administrative Instructions).
 - ☐ sheets which supersede earlier sheets, but which this Authority considers contain an amendment that goes beyond the disclosure in the international application as filed, as indicated in item 4 of Box No. I and the Supplemental Box.
 - ☐ (sent to the International Bureau only) a total of (indicate type and number of electronic carrier(s)) , containing a sequence listing and/or tables related thereto, in computer readable form only, as indicated in the Supplemental Box Relating to Sequence Listing (see Section 802 of the Administrative Instructions).

- This report contains indications relating to the following items:

- ☒ Box No. I Basis of the opinion
- ☐ Box No. II Priority
- ☒ Box No. III Non-establishment of opinion with regard to novelty, inventive step and industrial applicability
- ☒ Box No. IV Lack of unity of invention
- ☒ Box No. V Reasoned statement under Article 35(2) with regard to novelty, inventive step or industrial applicability; citations and explanations supporting such statement
- ☐ Box No. VI Certain documents cited
- ☐ Box No. VII Certain defects in the international application
- ☐ Box No. VIII Certain observations on the international application

Date of submission of the demand 24.10.2005	Date of completion of this report 06.12.2005
Name and mailing address of the international preliminary examining authority:  European Patent Office D-80298 Munich Tel. +49 89 2399 - 0 Tx: 523656 epmu d Fax: +49 89 2399 - 4465	Authorized Officer Strohmayer, B Telephone No. +49 89 2399-2669



**INTERNATIONAL PRELIMINARY REPORT
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Box No. I Basis of the report

1. With regard to the **language**, this report is based on the international application in the language in which it was filed, unless otherwise indicated under this item.
- ☐ This report is based on translations from the original language into the following language , which is the language of a translation furnished for the purposes of:
- ☐ international search (under Rules 12.3 and 23.1(b))
 - ☐ publication of the international application (under Rule 12.4)
 - ☐ international preliminary examination (under Rules 55.2 and/or 55.3)
2. With regard to the **elements*** of the international application, this report is based on *(replacement sheets which have been furnished to the receiving Office in response to an invitation under Article 14 are referred to in this report as "originally filed" and are not annexed to this report):*

Description, Pages

1-37 as originally filed

Claims, Numbers

1-35 as originally filed

Drawings, Sheets

1-8 as originally filed

- ☐ a sequence listing and/or any related table(s) - see Supplemental Box Relating to Sequence Listing

3. ☐ The amendments have resulted in the cancellation of:
- ☐ the description, pages
 - ☐ the claims, Nos.
 - ☐ the drawings, sheets/figs
 - ☐ the sequence listing (*specify*):
 - ☐ any table(s) related to sequence listing (*specify*):
4. ☐ This report has been established as if (some of) the amendments annexed to this report and listed below had not been made, since they have been considered to go beyond the disclosure as filed, as indicated in the Supplemental Box (Rule 70.2(c)).
- ☐ the description, pages
 - ☐ the claims, Nos.
 - ☐ the drawings, sheets/figs
 - ☐ the sequence listing (*specify*):
 - ☐ any table(s) related to sequence listing (*specify*):

* If item 4 applies, some or all of these sheets may be marked "superseded."

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Box No. III Non-establishment of opinion with regard to novelty, inventive step and industrial applicability

1. The questions whether the claimed invention appears to be novel, to involve an inventive step (to be non-obvious), or to be industrially applicable have not been examined in respect of:

☐ the entire international application,

☒ claims Nos. 29,31,33

because:

☐ the said international application, or the said claims Nos. relate to the following subject matter which does not require an international preliminary examination (specify):

☐ the description, claims or drawings (*indicate particular elements below*) or said claims Nos. are so unclear that no meaningful opinion could be formed (*specify*):

☐ the claims, or said claims Nos. are so inadequately supported by the description that no meaningful opinion could be formed.

☒ no international search report has been established for the said claims Nos. 29,31,33

☐ the nucleotide and/or amino acid sequence listing does not comply with the standard provided for in Annex C of the Administrative Instructions in that:

the written form

☐ has not been furnished

☐ does not comply with the standard

the computer readable form

☐ has not been furnished

☐ does not comply with the standard

☐ the tables related to the nucleotide and/or amino acid sequence listing, if in computer readable form only, do not comply with the technical requirements provided for in Annex C-*bis* of the Administrative Instructions.

☐ See separate sheet for further details

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Box No. IV Lack of unity of invention

1. ☒ In response to the invitation to restrict or pay additional fees, the applicant has:
- ☐ restricted the claims.
 - ☐ paid additional fees.
 - ☐ paid additional fees under protest.
 - ☒ neither restricted nor paid additional fees.
2. ☐ This Authority found that the requirement of unity of invention is not complied with and chose, according to Rule 68.1, not to invite the applicant to restrict or pay additional fees.
3. This Authority considers that the requirement of unity of invention in accordance with Rules 13.1, 13.2 and 13.3 is
- ☐ complied with.
 - ☒ not complied with for the following reasons:
see separate sheet
4. Consequently, this report has been established in respect of the following parts of the international application:
- ☐ all parts.
 - ☒ the parts relating to claims Nos. 1-28,30,32,34,35 .

Box No. V Reasoned statement under Article 35(2) with regard to novelty, inventive step or industrial applicability; citations and explanations supporting such statement

1. Statement

Novelty (N)	Yes: Claims	
	No: Claims	1-28,30,32,34,35
Inventive step (IS)	Yes: Claims	
	No: Claims	1-28,30,32,34,35
Industrial applicability (IA)	Yes: Claims	1-28,30,32,34,35
	No: Claims	

2. Citations and explanations (Rule 70.7):

see separate sheet

X1=A LeBail: "Monte Carlo indexing with McMaille", SSPD03, Sep.2003
X2=A.A.Coelho: "Indexing of powder diffraction patterns by ...", Feb.2003
A3=R.A. Jacobson: "A Monte Carlo method for indexing", 1997
A4=B.M.Kariuki et al.: "A new approach for indexing powder ...", 1999
A5=J.S.Hwang et al.: "XRAYSCAN: An Indexing Program ...", 1996
A6=R. Shirley: "Overview of powder-indexing program ...", Jul. 2003

Section IV

The common concept of independent claims 1,30,32 on the one hand and independent claims 29,31,33 on the other hand resides in

a method for determining the unit cell parameters of a crystalline solid form of a compound, which comprises providing a plurality of sets of unit cell parameters, one of which describes the correct values of the unit cell parameters of the crystalline solid form or values of the unit cell parameters that are proximate to the correct values of the unit cell parameters of the crystalline solid form.

This is the method performed by any conventional indexing program. Said common concept is thus anticipated by each cited document and thus not new, let alone inventive as required by Rule 13.1 PCT. The application contains the two inventions indicated in the search report.

Section V

1.1. The subject matter of independent method claim 1 (and of corresponding independent device claims 30,32) is anticipated by each of X1 or X2:

X1: title; page 9 entitled "What is examined in the automated 'black box' mode ?", in particular the increasing volumes indicated for each symmetry, for example "500-1000-1500-2000" for the "orthorhombic" symmetry etc. and the reduction of symmetry from top to bottom. See also the flow diagram on page 11 entitled " 'Simplicity' of the Monte Carlo algorithm in McMaille", in particular the steps "select crystal system", "define limits in volume and cell parameters" and "new crystal system ?".

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X2: the various symmetries are indicated in table 3; see Table 2, equation (3) and the sentence "part (b) of step (iv) gradually increases the volume V_1 according to ..." in the middle of the right column of page 87. See also the last sentence of the paragraph "2.1. Searching for the crystal system" on page 88: "On a 600 MHz personal computer, SVD-Index searches all crystal systems down to triclinic in approximately 3 min."

1.2. The argument that X1 and X2 use Monte Carlo methods to generate indexing solutions of a much larger space than is necessary does not hold good, since claim 1 is silent about the size of the search space.

Also the argument that X1 and X2 fail to teach reducing search space by considering molecular volume and symmetry does not hold good, since this reduction is not defined in claim 1 either.

2. Dependent claims 2-28, 34 and 35 are likewise anticipated or suggested by the cited documents (see passages indicated in the search report).

3. Dependent claims 21,23,26,28,34 and 35 are formulated in an unclear way ("a refinement method, which comprises providing results obtained from the method of claim ...") contrary to Art.6 PCT. A clear way would have been "a method as claimed in claim ..., further comprising a ... refinement of the results obtained by ...").